Nonlinear Iterations for Hydrostatic Equilibrium

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Outline

- Motivation
- Air-Water Equations
- Equilibrium Equations
- Numerical Results

Motivation

Multiphase flow models are used in subsurface studies to simulate the movement of fluids in a porous media environment.

- Oil-water simulation for reservoir modeling
- Black oil (three-phase) simulations
- NAPL remediation
- Groundwater flow in the unsaturated zone

The IPARS framework developed at CSM was developed to provide fast, accurate, three-dimensional simulations for each of the above.

Mass Balance

The mass balance equation for each of the α phases is given by

$$\phi \frac{\partial}{\partial t} (\eta \rho_\alpha S_\alpha) + \nabla \cdot (U_\alpha) = q_\alpha,$$

where U_α is given by Darcy's Law,

$$U_\alpha = -\rho_\alpha K \frac{k_\alpha}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha G \nabla D).$$

Advantages to Air-Water Formulation

- Consider both air and water phases
- Use data and splines to evaluate nonlinearities
- Use conservative algorithms for discretization
- Handle a variety of boundary conditions

Two-Phase Equations

Putting together the Darcy velocity and mass balance gives the two-phase equations

$$\frac{\partial}{\partial t}\left(\rho_\alpha \eta S_\alpha\right) - \nabla \cdot \left(\rho_\alpha k \frac{k_{r\alpha}}{\mu_\alpha}\left(\nabla p_\alpha - \rho_\alpha G \nabla D\right)\right) = q_\alpha,$$

where

$$\begin{aligned} \mu_\alpha &= \text{viscosity} \\ k_\alpha &= \text{relative permeability} \end{aligned}$$

The system is closed by including the saturation relationship

$$S_a + S_w = 1,$$

and the capillary pressure relationship

$$p_c(S_w) = p_n - p_w.$$

Density

The water phase is assumed to be slightly compressible; hence

$$\rho_w = \rho_0 \exp^{c_w(p_w - p_0)}$$

where c_w is the compressibility constant and ρ_0 and p_0 are reference densities and pressures.

The density for the air phase is obtained via the real gas law

$$\rho_a = \frac{p_a M}{Z(p_a)RT},$$

where R is the gas constant, M is the molecular weight of the gas, T is the temperature, and Z is the Z-factor.

Initialization

The reservoir is initialized by enforcing an equilibrium condition

$$\nabla p_\alpha - \rho_\alpha g \nabla D = 0.$$

This is done by using Newton loops to initialize both water and air pressures along with the water saturation.

The discretized equilibrium condition is

$$p_{i+1} - p_i - g\frac{1}{2}\left(\rho_i + \rho_{i+1}\right)\left(D_{i+1} - D_i\right) = 0.$$

Adjusting Density

The density for the water phase is

$$\rho_w = \rho_{w,ref} e^{c_w (p_w - p_{w,ref})}.$$

Thus

$$\begin{aligned}
\rho_{w,i+1} &= \rho_{w,ref} e^{c_w (p_{w,i+1} - p_{w,ref})} \\
&= \rho_{w,ref} e^{c_w (p_{w,i+1} - p_{w,i} + p_{w,i} - p_{w,ref})} \\
&= \rho_{w,ref} e^{c_w \Delta p_w} e^{c_w (p_{w,i} - p_{w,ref})} \\
&= \rho_{w,i} e^{c_w \Delta p_w}.
\end{aligned}$$

Newton Equation for Water Pressure Equilibrium

For equilibrium of water pressure, we have

$$F\left(\Delta p_w\right) = \Delta p_w - g\frac{1}{2}\rho_i\left(1 + \exp^{c_w \Delta p_w}\right)\left(D_{i+1} - D_i\right)$$

giving a Jacobian

$$F'\left(\Delta p\right) = 1 - \frac{g}{2} c_w \rho_{w,i} \Delta p_w \Delta D.$$

Initial Guess

The initial guess is found by assuming that

$$\rho_{w,i+1} \quad = \quad \rho_{w,i} + \left.\frac{\delta\rho_w}{\delta p_w}\right|_{p_w,i} \left(p^0_{w,i+1} - p_{w,i}\right),$$

which gives

$$\Delta p^0_w \quad = \quad \frac{g\rho w, i\Delta D}{1 - \frac{g}{2}c_w\rho_{w,i}\Delta D}$$

Air Phase Density

The Newton function for the air equilibrium condition is

$$F\left(p_{i+1}\right) = p_{i+1} - p_i - g\frac{1}{2}\left(D_{i+1} - D_i\right)\left(\frac{M}{RT}\right)\left(\frac{p_i}{Z(p_i)} + \frac{p_{i+1}}{Z(p_{i+1})}\right)$$

The initial guess for air equilibrium is based on the same assumptions, so that

$$p_{a,i+1} = p_{a,i} + \frac{\frac{g}{2}\Delta D \rho_{a,i}}{1 - \frac{g}{2}\Delta D \frac{M}{RT}\left(\frac{p_{a,i}}{Z_i}\right)}$$

Initialization for Saturation

The Newton function for the saturation initialization is

$$F(x) = p_c - p_{c,prev},$$

where $p_{c,prev}$ is fixed. The saturation is updated as

$$s_w = s_{w,prev} - \frac{F(x_{current})}{dp_c}.$$

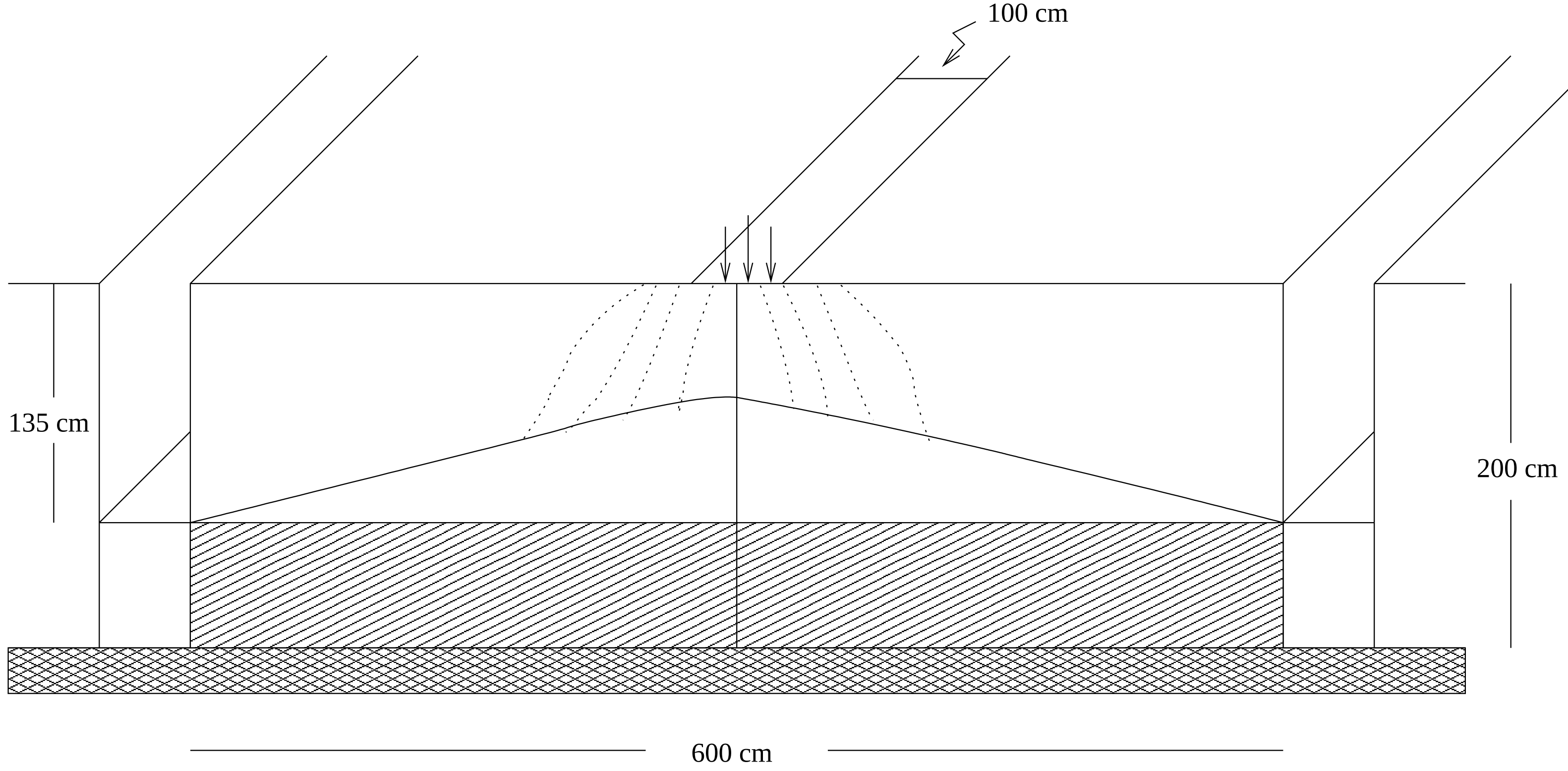
Spatial Discretization

- Cell-centered finite difference scheme
- Equivalent to the expanded mixed finite element method
  - Spaces are lowest order Raviart-Thomas spaces
    $(W_h, \boldsymbol{V}_h) \subset (W, \boldsymbol{V}) = (L^2(\Omega), \{\boldsymbol{v} \in H(div; \Omega), \boldsymbol{v} \cdot \nu|_{\partial\Omega} = 0\})$
  - Rectangular grid
  - References:
    - Russell, Wheeler (1983)
    - Arbogast, Wheeler, Yotov (1996, 1997)

Vauclin Test Problem

- Test problem from Vauclin, Khanji, Vachaud (Water Resources Research, 1979)
- Empirical and numerical results
- Transient
- Two-dimensional
- Vadose zone water table recharge

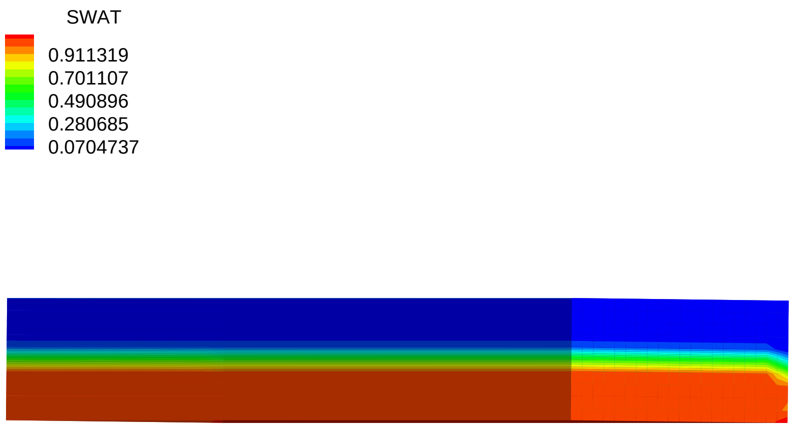
Test Domain

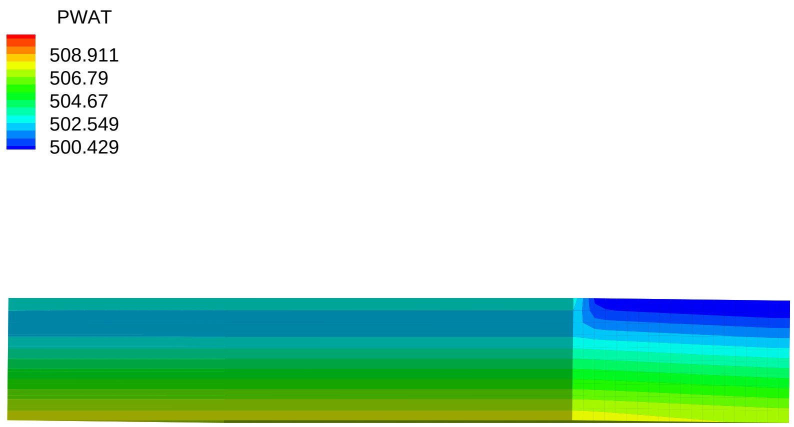


Water Saturation Data

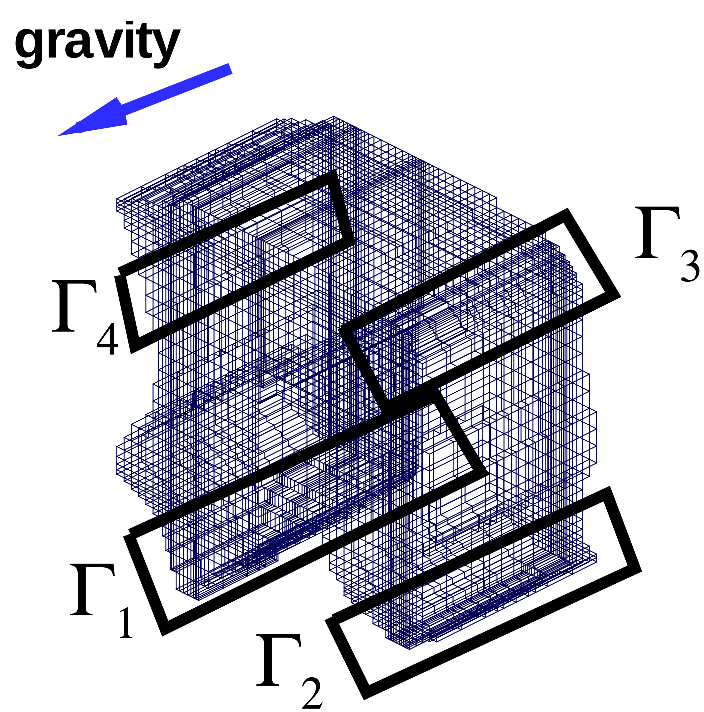
I / J =	1	5	9	13	20
1	.5750E-02	.5525E-02	.5525E-02	.5525E-02	.4023E-03
2	.7648E-02	.7647E-02	.7647E-02	.7647E-02	.5050E-03
3	.1235E-01	.1235E-01	.1235E-01	.1235E-01	.6782E-03
4	.3008E-01	.3008E-01	.3008E-01	.3008E-01	.1032E-02
5	.2043	.2043	.2043	.2043	.2158E-02
6	.9906	.9906	.9906	.9906	.4999
7	1.0000	1.0000	1.0000	1.0000	1.0000
8	1.0000	1.0000	1.0000	1.0000	1.0000
9	1.0000	1.0000	1.0000	1.0000	1.0000
10	1.0000	1.0000	1.0000	1.0000	1.000

Contours at Day 1

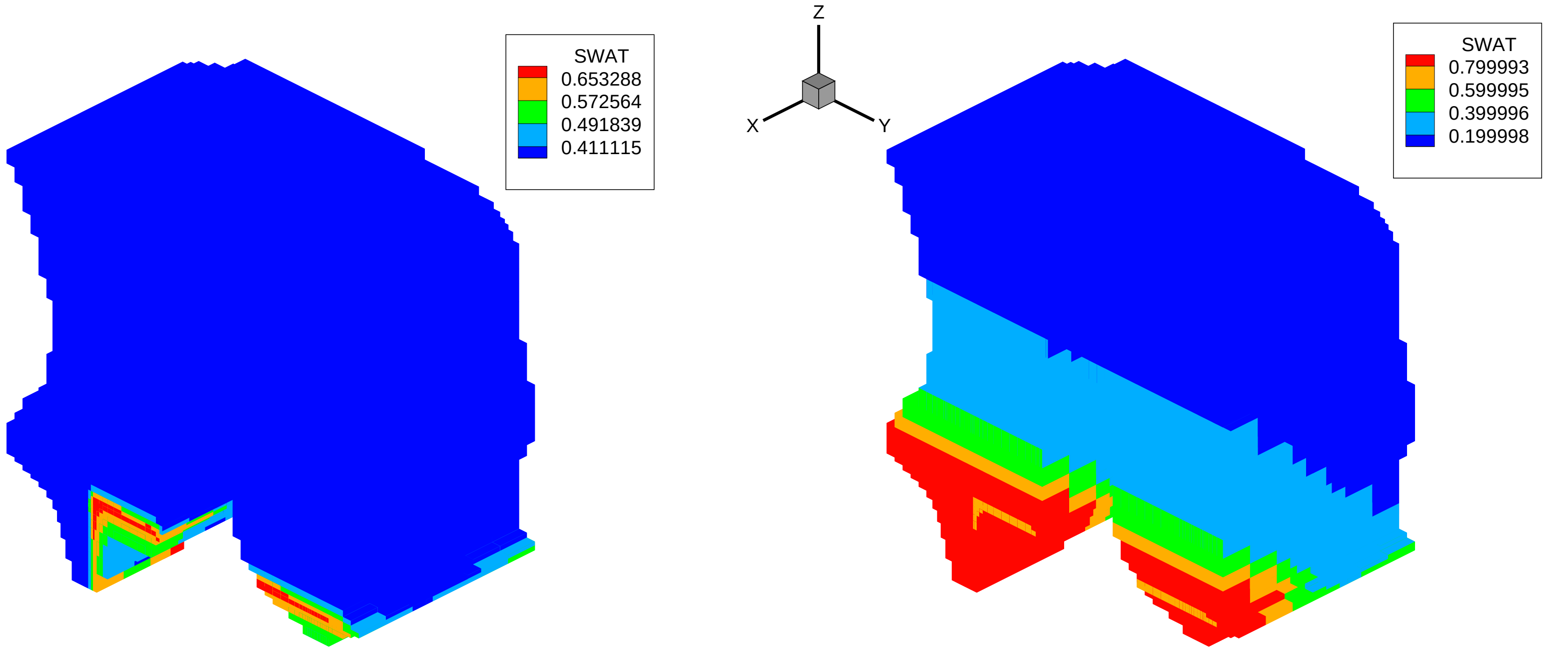




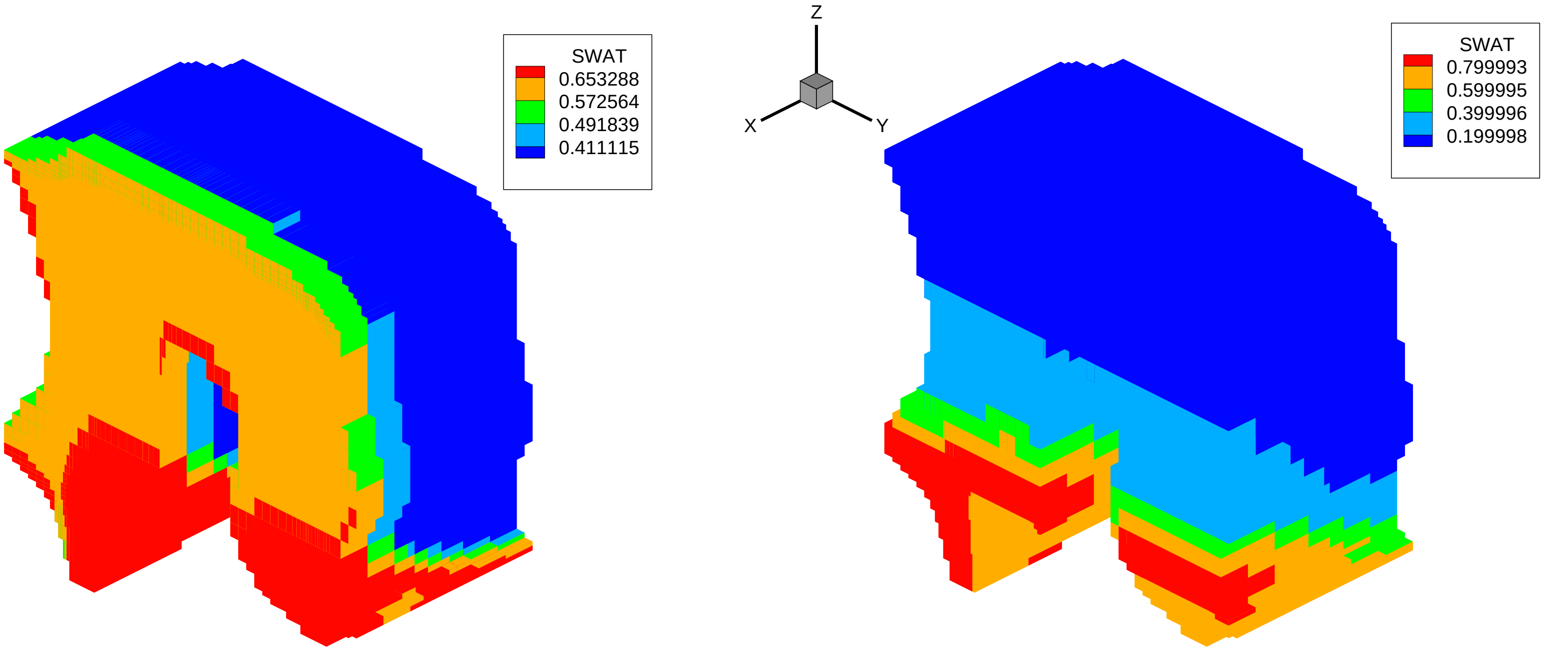
Oxbow Computational Domain



Saturations at Day 1



Saturations at Day 51



Saturations at Day 101